AOARD REPORT

The Institute for Material Science and Department of Material Science, Tohoku University, Sendai Japan, 2-3 Jun 94.

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P. McQuay
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Two labs were visited at the University of Tohoku: the Materials Design by Computer Simulation Laboratory of Professor Yoshiyuki Kawazoe, in the Institute of Materials Research ; and the Structural Materials Laboratory of Prof Hiroshi Oikawa, of the Department of Material Science. The Computer Simulation Lab, recently armed with arguably the most powerful supercomputer CPU in the world, and specifically configured to work material science and design problems, is attempting to position itself for a future leadership role in the field of computational material science. Professor Oikawa's Structural Materials Group continues to explore the high temperature deformation behavior of titanium alloys, with most of his current work aimed at understanding the high temperature deformation of the intermetallic compound, gamma TiAl. His results on the constitutive effect of microstructural features offer insight into improving the high temperature performance of this emerging class of structural materials.

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26 Jun 94

AOARD Trip Report

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SUBJECT: Trip Report - The Institute for Material Science and Department of Material Science, Tohoku University, Sendai Japan, 2-3 Jun 94.

1. ABSTRACT

Two labs were visited at the University of Tohoku: the Materials Design by Computer Simulation Laboratory of Professor Yoshiyuki Kawazoe, in the Institute of Materials Research ; and the Structural Materials Laboratory of Prof Hiroshi Oikawa, of the Department of Material Science. The Computer Simulation Lab, recently armed with arguably the most powerful supercomputer CPU in the world, and specifically configured to work material science and design problems, is attempting to position itself for a future leadership role in the field of computational material science. Professor Oikawa's Structural Materials Group continues to explore the high temperature deformation behavior of titanium alloys, with most of his current work aimed at understanding the high temperature deformation of the intermetallic compound, gamma TiAl. His results on the constitutive effect of microstructural features offer insight into improving the high temperature performance of this emerging class of structural materials.

2. OVERVIEW AND BACKGROUND

Tohoku University was one of the original Imperial Universities, the third in Japan, behind the University of Tokyo, and Kyoto University. The total research and teaching staff is estimated at 5,200, and the total number of students around 13,000. The University is located in several campuses in the city of Sendai, approximately 200 miles north of Tokyo. Sendai is the largest city, and considered the center of the six northern prefectures, called Tohoku, of the main island of Honshu. It is a beautiful city, nicknamed "mori no miyako," or the city of trees.

In the field of the physical sciences, there are many departments and research institutes at Tohoku University. These generally fall under one of the following organizations: the Faculty of Science; the Faculty of Engineering; The Graduate School Division of Engineering; The Graduate School Division of Science; or the Research Institutes. For instance, under the Research Institutes, are seven institutes including IMR, the Research Institute for Mineral Dressing and Metallurgy, the Research Institute for Scientific Measurements, the Institute of Fluid Science, etc. Additionally, there are three research institutes which are under the Faculty of Engineering, such as the Research Institute for Fracture Control. The combined capabilities and resources are immense, but the organization is rather diverse and complicated.

Tohoku University is believed by many to have the strongest overall material science program in Japan. Most of the key researchers work in IMR, although there are several key faculty in both the Faculty of Engineering and Science, as well as the Graduate Schools. A general overview of the IMR of Tohoku University, which was recently

published in the AOARD Asia Science Letter by Dr. Fujishiro, is attached (Atch 1). Also attached is the trip report of Dr. David Kahaner, who I accompanied on this trip (Atch 2). His report offers specifics on the new supercomputer system installed at IMR, as well as additional background information regarding IMR.

3. MATERIALS DESIGN BY COMPUTER SIMULATION LAB, IMR, 2-3 JUN 94
The impetus for the visit to IMR was an invitation by Dr. David Kahaner, currently with the ONR-Asia office, to visit the Materials Design by Computer Simulation Laboratory, headed by our host:

Professor Yoshiyuki Kawazoe.
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Kitahira 2-1-1
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The Computer Simulation Lab, has recently invested approximately $40M in three processor Hitachi S3800 supercomputer. The S3800 boasts the most powerful supercomputer CPU in the world, and with its purchase, IMR is attempting to position itself for a future leadership role in the field of computational material science. The supercomputing facility is dedicated for the use of IMR scientists, and specifically configured to work material science and design problems, with an impressive array of supporting computer and graphics equipment. As noted above, for details regarding the specific configuration and performance of the institutes new supercomputing facility, see the attached report by Dr. Kahaner.

My impression is that this laboratory is being built upon the *Field of Dreams* model: "If you build it, they will come." Dr. Kawazoe's group is a relatively new and unknown group in the world of computational material science, today. I would imagine with such an impressive facility, and the groups interest in attracting outside talent from around the world, the group will not remain in relative obscurity for long.

In addition to the group leader, Professor Kawazoe, we met with several of his research team. One of the distinguishing features of the group is the variety of computational material science problems which are being addressed. Below are listed their names, affiliations, and a brief description of their areas of research.

Assoc Prof Kaoru Ohno, permanent staff of IMR. Two of the theoretical projects are concerned with the behavior of Bucky Balls (BB): first, the electronic structure and interaction of BB molecular crystals at room and cryogenic temperatures; second, the structure of a BB molecular crystal deposited on a silicon substrate. The graphics which were produced to assist in visualizing these simulations were impressive, and they have found good agreement with experimental results.

Prof Krzysztof Parlinski, IMR Hitachi Chair, Inst of Nuclear Physics, Cracow, Poland. Simulation of the crystal structure of a high Tc superconducting material, looking at the interaction between annealing temperature, strain, and microstructure of the superconducting material.

Dr. Marcel Sluiter, visiting Assoc Prof, formerly with Los Alamos, and Prof Fu of Washington University. Simulation of typical structure and physical characteristics of alloys and intermetallics using the standard methods and algorithms: KKR, muffin tin, etc. Just beginning studies on Nb_3Al, in conjunction with Prof Hanada, also of IMR.

Dr. Xiao Hu, Asst Prof of IMR Simulating the magnetic behavior of several magnetic materials.

The supercomputer facility has only been operational since April of 1994, but has already produced several interesting simulations and studies. A description of these first studies are published, in part, in "The Science Reports of the Research Institutes of Tohoku University," Series A, Vol. 39, Dec 93. Examples of several of the papers by Professor Kawazoe's group are given below:

"The Orientational Influence on the Electronic Structure of the Solid fcc C_{60}"

"Classical MD Simulation and Ab-initio Mixed-basis Band Calculation of C_{60} Adsorbed on Si(100) Surface"

"Full-potential Mixed-basis Simulated Annealing Calculation of C_{60}"

4. STRUCTURAL MATERIALS GROUP, DEPT OF MATERIAL SCIENCE, 3 JUN 94
The following day I visited the main campus of Tohoku University, which is situated upon the top of the beautiful forested Mount Aoba (or Aobayama). My host was:

Prof Hiroshi Oikawa
Department of Material Science
Faculty of Engineering
Tohoku University
Aramaki-aza-Aoba
Aoba-ku, Sendai 980
Japan
Tel: 81 (22) 222-1800; Fax: 81 (22) 268-2949

Prof Oikawa explained that a typical national university in Japan, the Ministry of Education or Monbusho, provides approximately 1/3 of the laboratory operating expenses directly, about 1/3 of the operating expenses via competitive grants, and the remaining 1/3 of the funding comes from corporate or private grants or contracts. He commented that although some corporations often give grants with strings attached, that he has a policy not to accept such directed funds, but only accept grants where he has full control over the research and dissemination of information. In spite of this fact, he reported that his group still obtains adequate funding.

Prof Oikawa's group consists of an additional full Prof, Prof Kouichi Maruyama, Assoc Prof Jun-ichi Koike, and an Instructor, Dr. Hioyuki Sato. The group currently has 10 graduate students, at least three of which are pursuing PhD's. The emphasis of the group is high temperature deformation of metals, or more specifically, studies of compression creep on crystalline materials. The major research themes are:

- Deformation of Cubic Solid Solutions at Elevated Temperature
- Deformation of Hexagonal Alloys at Elevated Temperature
- Creep of Intermetallics

- Superplasticity of Advanced Materials
- Deformation of Carbon Composites
- Alloy Design of Heat-Resisting Materials
- High Temperature Strength of Titanium Alloys
- Structure and Strength of Fine-Scale Advanced Materials

The primary research tool of choice are home-made load controlled compression creep frames. The laboratory is also equipped with several servo-hydraulic frames. The majority of the creep testing is conducted in air or flowing argon. Although the equipment was rather unimpressive, I was impressed with the care taken in producing homogeneous and well characterized materials for testing and analysis.

The material systems his group is currently working on includes Ti alloys, TiAl, Ti_3Al, Al alloys and composites, Mg alloys, Fe and steel alloys, Si, and Ni_3Al. The largest current project is creep behavior of gamma TiAl.

Prof Oikawa has generated considerable controversy with his work on the creep properties of gamma TiAl. There are at least three controversies which I am aware of. The first deals with the applicability of compression creep deformation to the more typical tensile creep conditions found in most structural applications, such as turbine or compressor blades. The issue revolves around a still unresolved issue regarding a possible tension-compression anisotropy in gamma TiAl.

The second controversy is Prof Oikawa's remarks concerning the inherently poor creep strength of gamma TiAl, which most everyone in the community has taken to be slanderous, in spite of little evidence to support either side of the argument, as very little work in the creep of TiAl has been done. If nothing else, Prof Oikawa's provocative claims have hopefully motivated the community to study the high temperature properties of this potential high temperature material.

The last controversy involves Prof Oikawa's research on single phase model systems. The early work on the titanium-aluminum system by Prof Oikawa's group concentrated on the creep behavior of single phase TiAl. This work had been criticized by some in the scientific community because it was conducted on single phase material, which currently has little commercial interest because of it's poor combination of room temperature strength, fracture toughness, and ductility. Several years ago, his group began a study of the creep behavior of single phase Ti_3Al, which also encountered similar criticism.

The work on the each of the two constituent phases which makes up the two phase gamma alloys, TiAl and Ti_3Al, is nearly complete. His group is now studying the creep behavior of the commercially interesting two phase alloys, to understand the salient microstructural and metallurgical features which dominate the creep behavior of these materials. Understanding the entire metallurgical system of the two phase alloys should be greatly aided by the understanding gained on the behavior of the constituent phases. This information should be very valuable in formulating improved alloy and microstructural combinations with improved high temperature strength and creep resistance.

In particular, preliminary results indicate that the largest contribution to the improvement in creep resistance of the Fully Lamellar microstructure in the low strain rate, low stress creep region, is the coarse grain size, and not the lamellar structure itself, or the interlocking grain boundaries found in some lamellar microstructures. These features appear only to play a large effect at high stress/strain rate conditions. These results are planned to be published

first in the Proceedings of the International Symposium on Gamma Titanium Aluminides '95 (Las Vegas, Nevada, Feb 95).

Prof Oikawa is the Chairman of the Organizing committee for the Tenth International Conference on the Strength of Materials, to be held in Sendai, 21-26 Aug 94. The stated purpose of the conference is to "provide an opportunity to exchange intimately our knowledge and deepen our understanding of fundamental aspects of the strength of materials..." Over 300 contributed papers have been received from 21 countries. More information regarding the conference can be obtained by writing or faxing Prof Oikawa at the numbers above.

5. SUMMARY AND COMMENTS

As mentioned previously, although the laboratory of Prof Kawazoe is relatively new and unknown, it is a unique facility with one of the most powerful supercomputers in the world at the disposal of a single research institute, and primarily, a single research group. The laboratory has a tremendous potential to attract talent from all over the world, and become a premier center for computational material science.

Prof Oikawa continues his important, and often controversial research on the creep behavior of crystalline materials. The issue regarding Prof Oikawa's reliance on compressive creep testing, and it's applicability to tensile creep behavior remains an open issue. However, regardless of ones conclusions, the controversy stirred by his comments regarding the poor inherent creep resistance of gamma may have the desired effect: "One of the challenging problems for developing practical materials based on intermetallics in the Ti-Al system is how much materials scientists/engineers can improve the strength by metallurgical means." (K. Maruyama, and H. Oikawa, Mat. Res. Soc. Symp. Proc. Vol. 288, p. 653, 1993.) Clearly this is an area in the development of gamma TiAl alloys which has been ignored for too long.

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ABSTRACT. Titles from Science Reports, RITU, Ser.A, Vol 39, No.1, "Materials Design by Computer Simulation I -- Physics and Chemistry of Nanoscale Materials", ed Prof Y.Kawazoe, 12/93.

Institutes at Tohoku University (Sendai Japan) have developed a significant computational capability. This year Tohoku has added a four processor NEC SX-3 and a three processor Hitachi S3800, making it one of the best endowed universities in the country. A major activity is in materials research. What follows are the titles from Tohoku's Science Reports, RITU, Ser.A, Vol 39, No.1, "Materials Design by Computer Simulation I -- Physics and Chemistry of Nanoscale Materials", ed Prof Yoshiyuki Kawazoe, and published in English, 12/93. Information about these papers can be obtained from me, or by writing either directly to Prof Kawazoe, or to Prof Hiroshi Komatsu at the following address

Institute for Materials Research
Tohoku University
Sendai 980 Japan

PREFACE

Computer simulation is one of the most rapidly advanced research fields on various subjects. Especially, it is widely accepted that the most heavy users of the present supercomputers are the researchers in materials design and fluid dynamics. It is really the case in Tohoku University; in this year, our Institute is selected to be financed by the Government for a new supercomputing system, as the third case in Tohoku University, after the Main Computer Center and Institute of Fluid Science.

It is a great pleasure to start this series of the Science Reports, RITU, on the materials design by computer simulation at this prominent time. Before this plan for the publication of RITU, we have already held three symposiums on "Physics and Chemistry of Nanoscale Materials" in Sendai headed by Professor Tamotsu Kondow with the University of Tokyo. Every year we had two days of meeting with about 40 participants of theoretical and experimental backgrounds. The first issue of this series starts including the reports of the last symposium held on 30th of November and 1st of December, 1993.

The last aim of this series is to gather and distribute efficiently the

everlasting human activity to search fundamentally new materials by using up-to-date computer simulation technologies based on the advanced theoretical approaches. The object contains not only nanoscale materials but also complex bulk materials in practical use. The large variety of the subjects on materials design by computer simulation encourages us to issue this series of RITU in the nearest future.

December 1993, Responsible Editor, Yoshiyuki Kawazoe

Sci. Rep. RITU, A-Vol.39, No.1 (December, 1993)
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LABORATORY PROFILE

1. Institute for Materials Research, Tohoku University

At Tohoku University, there are six physical science research laboratories in the areas of physical science, namely, the Institute of Materials Research (IMR), the Research Institute of Electrical Communication, the Research Institute for Scientific Measurements, the Institute for Advanced Materials Processing, the Institute of Fluid Science and Mechanics and the Institute for Chemical Reaction Science. Among these laboratories, IMR is the largest and its research activities are of particular interest to the Air Force.

Statistics:
Location: 2-1-1 Katahira, Aoba-Ku, Sendai 980, Fax 81 (022) 215-2182
Established: 1917 Lab. Director: Prof. Kenji Suzuki
No. of Employees: 269 No. of Professionals: 151
Budget (1994): $41M

When it was established, the laboratory was called the Institute of Iron, Steel and Other Metals in both Japanese and English, but recently they changed the English name to IMR. There are 54 professors and associate professors. Historically, their research emphasis has been on electromagnetic materials and their physical properties, and the physical metallurgy of alloy system. They have, in recent years, broaden their endeavor to include all aspects of the electronic, magnetic, magneto-optical, and mechanical properties of advanced materials. The laboratory is known worldwide for the Suzuki effect, the theoretical work on dislocation/solute interactions (former professor, H. Suzuki), and the so-called Yajima process in preceramic polymer, e.g., Nicalon SiC fiber (late professor S. Yajima), and the ductalizing effects of boron on Ni Aluminide (former professor, O. Izumi). Their research works are, in addition to regular scientific journals, selectively published on *Tohoku University Kenkyu Hokoku* (in Japanese) and some of the topics are also collectively published on *Science Reports of Research Institute, Tohoku University* (in English), Series A.

Among the notable research topics and leaders presented in these reports in 1993 are (1) nonequilibrium phase/amorphous alloys (T. Masumoto and A. Inoue), (2) functionally gradient materials (T. Hirai), (3) computational designing of new alloys and ceramics (Y. Kawazoe), (4) magneto-optics/giant magneto resistance (H. Fujimori) and (5) magnetic phase transition/high Tc ceramic superconductor (M. Hiraki).

The budget looks extremely small for the size of the laboratory and the scope of the activity. According to our conversation with the professors there, however, like the laboratories and science and technology departments of the other national universities, they take graduate students and trainees from the industries whose donations and contributions for the operation and new facilities are enormous and may match the regular budget. (Shiro Fujishiro)